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In the following we give an overview of the work completed under the grant AFOSR-84-0315 entitled "Continuation and Multi-grid Methods for Bifurcation Problems" since October 1, 1984. The research under that grant concerns the numerical solution of bifurcation and nonlinear eigenvalue problems for parameter-dependent partial differential equations and systems. The scope of the research is rather wide, stressing the development, study and implementation of computational methods for several classes of difficult nonlinear problems, but, also including the derivation of analytic results in cases where these questions had not been settled before. The work under the grant has resulted in 26 papers in refereed journals or refereed proceedings volumes of major conferences; they are listed at the end of this section.

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Continuation and Multi-grid Methods
for
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1. Accomplishments under the Current Grant

In the following we give an overview of the work completed under the grant AFOSR-84-0315 entitled "Continuation and Multi-grid Methods for Bifurcation Problems" since October 1, 1984. The research under that grant concerns the numerical solution of bifurcation and nonlinear eigenvalue problems for parameter-dependent partial differential equations and systems. The scope of the research is rather wide, stressing the development, study and implementation of computational methods for several classes of difficult nonlinear problems, but, also including the derivation of analytic results in cases where these questions had not been settled before.

The work under the grant has resulted in 26 papers in refereed journals or refereed proceedings volumes of major conferences; they are listed at the end of this section. The following section gives an overview of the various results.

2. Two Major Areas of Completed Research

A rough classification of the research completed under the current grant would identify two major areas given below together with the resulting publications.

(1) Development of computational methods for and study of free boundary problems for partial differential equations. [1, 7, 8, 9, 11, 13, 14, 17, 20, 21, 23]

(2) Efficient numerical solution and continuation for systems of nonlinear partial differential equations. [2, 3, 4, 5, 6, 12, 15, 16, 18, 19, 22, 24, 25, 26]

While there is a clear cut between the classes of problems in (1), free boundary problems usually described by variational inequalities, and (2), systems of nonlinear partial differential equations with various boundary conditions, the approaches used and the techniques developed are similar in several instances. Bifurcation of solutions with respect to a parameter, an important phenomenon in many applications presently of interest, is considered both in (1), [1, 7, 11, 14, 20] and in (2), [2, 3, 4, 6, 12]. Continuation along solution curves or on solution manifolds has been studied both practically and theoretically, for the problems from (1) in [8, 9, 11, 14, 17, 23] and for those from (2) in [2, 4, 5, 6, 15, 18]. Finally, multi-grid algorithms representing the most efficient methods for the solution of partial differential equations have been developed and implemented for the boundary problems (2) in [2, 5, 6] and, for the first time also for the variational inequalities from (1) in [13].

The following two sections deal in more detail with the problems and results listed above under (1) while the subsequent sections are concerned with the area (2) partly overlapping with (1) in the last two sections.

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2.1 Continuation for Variational Inequalities

Formally, a variational inequality may be written in the form $I_\lambda'[u](v - u) \geq 0$, where I_λ, for example, denotes the total energy of a physical system and u its state. If u could attain arbitrary values then the first variation of the energy functional was zero in the solution u_0, $I_\lambda'[u_0] = 0$ and a variational equality and corresponding (Euler-Lagrange) differential equation would result. In case, however, that the state can only vary under certain constraints, formally denoted by $u \in K$, then the above inequality defines the solution $u = u_0$ if it holds for all $v \in K$.

In the case that the functional in the above inequalities does not depend on one or several parameters λ the numerical solution of the associated variational inequalities had been under research earlier, in particular also by the principal investigator. In particular, efficient computational methods as preconditioned conjugate gradient [27] and multi-grid algorithms [28] had been successfully applied. Under the present grant parameter-dependent variational inequalities were one of the major focal points. Typically, the functional then has the form $I_\lambda[u] = f(u) - \lambda g(u)$, where f, g represent different components of the energy and λ usually stands for a physical parameter that acts as a force or a load. In the resulting variational inequality this λ enters as eigenvalue parameter, making the resulting problem a nonlinear eigenvalue problem. It is nonlinear in two different ways. Even if f, g were quadratic functionals and the corresponding Euler-Lagrange equation linear for arbitrary u, the fact that only $u \in K$ is admissible makes this problem a nonlinear one. In addition, the functionals f, g are in general not both quadratic yielding a second form of nonlinearity.

One of the very first papers on continuation for variational inequalities is [8]. At that time there had only very few papers appeared on this subject at all, from a group of French mathematicians [29, 30, 31] While several numerical methods were applied to a special class of second order semilinear variational inequalities in [31], they could not be justified theoretically. The method of [8] can be analyzed by generalizing earlier results of the principal investigator. Through the extensive computations in [8] also a phenomenon was detected and successfully dealt with ('spurious transition points') that had been overlooked in the earlier work.

The results and observations from [8] were the starting point for a series of further investigations largely together with one of our collaborators. A lengthy study with the French group is given in [9], while theoretical and practical results which go well beyond these are presented in [11, 14, 17, 23]. For the sake of brevity it may suffice here to say that

a different technique of proof, variational as opposed to fixed-point arguments, permitted a substantial generalization of the class of problems considered. Secondly, the numerical methods developed in [8] and refined and justified in [14, 17] are more powerful than what had been used so far.

2.2 Bifurcation and Multi-grid for Variational Inequalities

The problems described in the previous section are some of the computationally most involved ones in the context of partial differential equations. While, naturally, in first approaches to various aspects of these problems not the most complex example from the applications was chosen, the latter represent the ultimate goal of our work. Continuation along solution manifolds of variational inequalities necessitates the solution of a series of highly nonlinear problems. It is thus desirable to utilize the most efficient methods available. The first development and application of multi-grid algorithms for the class of variational inequalities considered in [8, 9] could be reported in [13]. While a theoretical analysis of the method proposed in [13] could not yet be completed, the numerical results of [8, 17] served as benchmarks to validate the computational procedure.

The problem of bifurcation of solutions is relatively well understood in the case of partial differential equations. Much less is known for variational inequalities. Together with one of the experts in the analytical study of this phenomenon we have been able to settle already several open questions. Of interest are, for example, variational inequalities describing the deflection of mechanical objects (beams, plates, shells) subject to constraints in the form of obstacles. While branching takes place at the critical load parameter, as is well-known, the open question is for which load the object after subsequently contacting the obstacle starts to lift off again ("snapthrough"). This represents a secondary bifurcation point in a non-standard framework, however. For beams, and different plates the answer could be given in [1, 7, 20, 23]. Numerical analysis and computations were crucial in all those papers.

2.3 Bifurcation for Systems of PDE's

In the previous section the term bifurcation was used in the narrow sense that for certain values of the physical parameters of a system a branching occurs, i. e. the state may follow several paths on a solution manifold. The mathematical model describing the system in general contains all possible states while the actual physical development—which branches are followed—depends on physical imperfections, perturbations, or the history of the process. Frequently the term bifurcation is already used when there is a non-uniquenss of solutions,

due, for example, to fold-points along the solution branch and continuation methods have to be used to overcome these difficulties. While these latter methods will specifically be addressed in the next section, here we are concerned with other aspects of bifurcation problems.

An important class of bifurcation problems is that where at a bifurcation point from the primary branch secondary branches of solutions bifurcate along which these solutions exhibit less symmetry than those on the primary branch. A method for boundary value problems developed earlier by the principal investigator in [32](generalized inverse iteration), was extended to such problems in [33]. While the example considered there was rather simple, a more complex application showing the power of the approach was studied in detail in [3].

One of the many interesting aspects of parameter-dependent PDE's is the fact that their discretizations exhibited spurious solutions. In addition to solutions which for finer and finer discretizations converge to the solutions of the original continuous problem, there are branches of solutions that do not correspond to "real" solutions and which disappear if the discretization is refined. For the well-known Bratu problem: – Laplacian $(u) = \lambda e^{u}$ with homogeneous Dirichlet boundary conditions no bifurcation (in the narrow sense of the word) occurs for the continuous solution while spurious solutions may branch off a relevant solution curve. This situation was addressed in [6].

2.4 Continuation and Multi-grid for PDE's

Many nonlinear PDE problems of interest in the applications in areas as diverse as solid mechanics, continuum mechanics, solid state electronics, etc., are parameter-dependent and continuation is necessary to obtain the desired solutions. It is thus natural that computational methods for this purpose are not only developed and analyzed but also implemented in software packages which are given to engineers and scientists whose response and experience with them then serve as a feedback to the mathematician to reconsider and refine his approaches. While the parameter-dependent problems requiring continuation can formally be written as $G(u, \lambda) = 0$, where u denotes the state variables and λ the parameters, in this and the previous section we were assuming that G stands for a system of nonlinear partial differential equations, i.e., u is a vector function, the number of components being equal to the dimension of the system. For an important class of second order PDE's a novel continuation technique was given and analyzed in [2, 4, 5, 6]. The differential equation is of general divergence from and includes many examples from the application areas listed above. While details of the method in the scalar case (systems of dimension 1) are given in [2, 4], three-dimensional systems, in particular that from VLSI

device simulation were considered and solved in [5]. The continuation method was implemented in the multi-grid finite element package PLTMG [34]. This package is widely used in industry and research labs. A further development of the continuation method, affecting both the "predictor" and the "corrector" steps, was accomplished in [15] and implemented in the latest release of the package [35].

2.5 Differential Equations on Manifolds

Recently first results were obtained for a more general class of PDE problems than considered in the previous two sections. In the case of, say, a PDE on a two-dimensional domain, the solution above was assumed to have the form $u(x, y)$, (x, y) being a point in the domain of definition. In this case u is a univalued function of the spatial variables and may be graphed accordingly. We address now a class of problems where this does not hold anymore. The differential equation is again of second order but the solution has to be written as $(u, v, w) \in \mathbf{R}^3$ and has to be parametrized by writing each of its components as a function of a variable in a two-dimensional parameter-domain, i.e. $u = u(r, s)$ etc. The solution is thus a general 2-manifold in 3-space. One example, which is only coincidentally also of interest to mathematicians, namely differential geometers, is that of capillary surfaces. The problem is to determine the liquid-liquid or liquid-gas interfaces of amounts of liquid that are confined to some container. Here, container has to be understood in a very general way; it may, for example, be a plane on which a liquid drop sits or from which it is pending.

The capillary surface problem is of great interest to physicists and engineers, also, but not only in situations where experiments are difficult and costly as in a micro-gravity environment (semiconductor production in space, etc.). A breakthrough in the computational solution of these and thus similar problems using a finite element method and utilizing continuation with respect to the parameters of the problem was made in [16, 18, 22]. These results were deliberately sent to journals in the appropriate areas of applications to reach that audience. For the sake of brevity we do not give details of the results here. Suffice it to say that in this context also bifurcation (in the narrow sense) but also multiplicity of solutions due to hysteresis effects etc. occur.

2.6 Bifurcation in Interface Problems

While the results and the algorithms presented in [16, 18] represent a breakthrough in the approximation of interface problems they only touch on the class of problems that now may be attacked using this new approach. The long-range goal will be to solve time-dependent

problems involving both capillary and flow phenomena. Very little work has been done in this area since the adequate computational treatment of each of those aspects separately still represents a formidable task. But, in the combination a presently untractable difficulty arises. While only recently satisfactory results could be obtained for the computational solution of the Navier-Stokes equations in fixed three-dimensional domains, the problems considered here would always involve a free boundary. This boundary would, in fact, only be determined through the coupling of the flow and the capillary effects.

The principal investigator recently started a cooperation with Profs. G. P. Neitzel and D. P. Jankowski from the Department of Mechanical and Aerospace Engineering at Arizona State University. This work is on the stability and instability of thermocapillary convection in models of the float-zone process. It is a pioneering project on the important stability questions of the process used to grow crystals for semiconductors both in a terrestial setting, but in particularly for its planned utilization in space. In this technique a poly-cristalline rod is moved slowly through a heating device which melts a portion of the rod. Ideally, this melt re-solidifies to form a single crystal, which is then used as a substrate for building micro-electronic devices. Since surface tension forces must support the zone, the rise of the revolving crystal is limited in earth-based production. In fact, the surface tension and density of some materials, e. g., gallium arsenide, are such that crystals of useful size cannot be grown on earth by the float-zone process. Crystals grown by this method exhibit undesirable non-uniformities in material properties and considerable effort has been motivated by the idea that the implementation of the process in a micro-gravity environment, such as exists on the Space Shuttle, can eliminate, or at least drastically reduce, these problems. Since experiments in a micro-gravity environment as, e. g., on the Space Shuttle, are expensive and very limited it is extremely important to develop computer simulations in order to facilitate space-based crystal growth for solid state electronics purposes.

The first completed papers on this subject are [24, 25, 26]. They show that the computational procedures proposed there are efficient and robust. In cases where results from model experiments exist excellent agreement was found. The techniques of [24, 25, 26], however. allow now the computation of the physically relevant cases, in particular low to zero gravity and crystal material as silicon. The model experiments had used other substances in order to be able to visualize the flows. The main result of the papers [24, 25, 26] was an energy stability bound for the Marangoni convection for wide ranges of the physical parameters. A region of stability and safe production could be identified which lies below (in terms of Marangoni number) the first (Hopf) bifurcation point of the underlying Boussinesq equations.

2.7 Publications Completed under the Grant

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2. H. D. Mittelmann, Multi-level continuation techniques for nonlinear boundary value problems with parameter-dependence, Appl. Math. Comp. 19, 265-282 (1986).
3. H. D. Mittelmann, B. Thomson, An algorithm that exploits symmetries in bifurcation problems, Notes on Numer. Fluid Mech. 16, 52-68 (1987).
4. H. D. Mittelmann, A pseudo-arclength continuation method for nonlinear eigenvalue problems, SIAM J. Numer. Anal. 23, 1007-1016 (1986).
5. R. Bank, H. D. Mittelmann, Continuation and multi-grid for nonlinear elliptic systems, in "Multigrid Methods II", W. Hackbusch, U. Trottenberg (eds.), Springer Lecture Notes in Mathematics, vol. 1228, 1986.
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7. E. Miersemann, H. D. Mittelmann, A free boundary problem and stability for the circular plate, Math. Meth. in the Appl. Sci. 9, 240-250 (1987).
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19. H. D. Mittelmann, Nonlinear parametrized equations: new results for variational problems and inequalities, to appear in AMS Lectures in Applied Mathematics series.

20. E. Miersemann, H. D. Mittelmann, A free boundary problem and stability for the rectangular plate, to appear in Math. Meth. in the Appl. Sci.

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24. Y. Shen, G. P. Neitzel, D. F. Jankowski, and H. D. Mittelmann, Energy stability of thermocapillary convection in a model of the float-zone crystal-growth process, submitted to J. Fluid Mech.

25. H. D. Mittelmann, Computing stability bounds for thermocapillary convection in a crystal-growth free boundary problem, to appear in ISNM, Birkhäuser-Verlag, Basel and Boston.

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Research and Teaching Interests:

Numerical solution of partial differential equations; finite elements; large-scale scientific computation for linear and nonlinear problems; multi-grid and other fast solution methods; numerical solution of bifurcation problems.

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University of Mainz	1971-1973	Scientific Staff, Computing Centre
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University of Dortmund	1977-1984	Associate Professor/Professor
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Society for Industrial and Applied Mathematics, Deutscher Hochschulverband, member of the GAMM activity groups "Discretization Methods in Solid Mechanics" and "Efficient Numerical Methods for Partial Differential Equations".

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Continuation and Multi-grid Methods for Bifurcation Problems, AFOSR 84-0315 (10/1/84–11/30/89, $250,000, PI).

Exploring and Controlling Spatio-Temporal Chaos and Complex Structures through Visualization: A Mini Super-Computer Approach, AFOSR 89–0155, DURIP, (12/1/88, $269,133, co-PI).

Stability and Instability of Thermocapillary Convection in Models of the Float-Zone Process, NAG 3-1054 NASA, Microgravity Science & Applications Division (6/15/89–6/14/91, $480,000, co-PI)

Spatio-Temporal Complexity and Large Scale Structures in Problems of Continuum Mechanics, AFOSR (URI), (7/1/89–7/15/92, $1,251,776, co-PI).

Continuation and Multi-grid Methods for Bifurcation Problems, proposed to AFOSR (12/1/89–11/30/92, $268,590, PI).

Selected invitations to conferences

1985 Second Copper Mountain Conference on Multigrid Methods, Copper Mountain, Colorado.
Second European Conference on Multigrid Methods, Cologne, Germany.

1986 Efficient numerical methods in continuum mechanics, Kiel, Germany.
Conference on nonlinear pde's, Salt Lake City, Utah.
First World Congress on Computational Mechanics, Austin, Texas.
AMS Regional Meeting, Logan, Utah.
Finite Elements in Continuum Mechanics, Oberwolfach, Germany.

1987 Third Copper Mountain Conference on Multigrid Methods, Copper Mountain, Colorado.
ASU Miniconference on Optimization, Tempe, Arizona.
AMS-SIAM Summer Seminar on Computational Aspects of VLSI Design, University of Minnesota.
German-U.S. American Workshop on New Applications and Algorithms for Optimal Control and Parameter Identification, Trier, Germany.
Annual Dutch Seminar on Numerical Mathematics. Woutschoten, Netherlands.
Multigrid Methods, Oberwolfach, Germany.

1988 AMS-SIAM Summer Seminar on Computational Solution of Nonlinear Systems, Fort Collins, Colorado.
Recent Trends in Nonlinear Computational Mathematics and Applications, University of Pittsburgh.
Fundamental Problems in Mechanics, Leipzig, Germany.
Bifurcation Theory and its Numerical Analysis, Xi'an, PR China.
Mathematical Modeling and Simulation of Electric Circuits, Oberwolfach, Germany.
Numerical Treatment of Problems in Solid Mechanics, Bad Honnef, Germany.

1989 Fourth Copper Mountain Conference on Multigrid Methods, Copper Mountain, Colorado.
SIAM Annual Meeting, San Diego.
Computational Methods in Solid Mechanics, Oberwolfach, Germany.
Free Boundary Problems, Numerical Treatment and Optimal Control, Oberwolfach, Germany.
Computation of Nonlinear Flow and Instabilities, Austin, Texas.
Workshop on Continuation and Bifurcations: Numerical Techniques and Applications, Leuven, Belgium.
Miniconference on Newton-like Methods for Large-Scale Nonlinear Methods, Logan, Utah.

1990 Fourth International Conference on Computational and Applied Mathematics, Leuven, Belgium
Contributions to the Numerics of Partial Differential Equations, Darmstadt, Germany
Multigrid Methods, Oberwolfach, Germany

<u>Conferences/Sessions organized</u>

1980 Bifurcation Problems and Their Numerical Solution, Dortmund, Germany.
1983 Numerical Methods for Bifurcation Problems, Dortmund, Germany.
1985 SIAM Fall Meeting, Tempe, Arizona.
1986 Continuation Methods and Algorithms, minisymposium at SIAM National Meeting, Boston.
1987 Nonlinear Parametrized Equations, minisymposium at ICIAM 87 meeting, Paris, France.
Nonlinear parameter dependent pde's and their effective solution, Tempe, Arizona.
1989 Nonlinear Problems in PDE's, minisymposium at SIAM National Meeting, San Diego

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PUBLICATIONS OF HANS D. MITTELMANN

1. Die Approximation der Lösungen gemischter Randwertprobleme quasilinearer elliptischer Differentialgleichungen, Computing 13, 253-265 (1974)

2. Finite-Element Verfahren bei quasilinearen elliptischen Randwertproblemen, in "Numerische Behandlung nichtlinearer Integrodifferential- und Differentialgleichungen", R. Ansorge, W. Törnig (eds.), Springer Lecture Notes in Mathematics, vol. 395, 1974

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